Gap formation and phase diagram of the disordered Hubbard model in the alloy-analogy approximation

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We study the gap for one-particle excitations as a function of the on-site repulsion U and the disorder W in the disordered Hubbard model in two and three dimensions. We consider the half-filled band case in the paramagnetic phase of this model. The analysis is done within the alloy-analogy approximation using the localized-eigenstates approximation to calculate the density of states. We find that there is a critical U_c for a gap opening at the Fermi level in both two and three dimensions. This allows us to determine a phase diagram of the model that separates a Mott-Hubbard insulating phase and an unspecified gapless phase. The critical U_c line grows with disorder and tends to be linear for large enough W. Our results are consistent with previous real-space renormalization-group studies.

The Hubbard Hamiltonian[1] is a standard model in the study of strongly correlated electronic systems. Although it attracted much attention in the past as a model for narrow-band metals, it is not yet fully understood. Nowadays, it has attracted a renewed interest as a model for the electronic properties of the high-T_c superconductors discovered by Bednorz and Muller.[2,3]

The Hubbard model reads

$$H=\sum_{i,\sigma} E_i n_{i\sigma}-\sum_{\substack{i,j\\ \sigma}} T_{ij}(c_{i\sigma}^{+}c_{j\sigma}+\text{H.c.})+\sum_i U n_{i\uparrow}n_{i\downarrow}\ , \quad (1)$$

where E_i is the binding energy of one electron at site i, t_{ij} is the intersite hopping energy, usually taken between nearest neighbors and site independent, and U is the on-site repulsion energy. In the presence of disorder, E_i is a random site-dependent energy, with some probability distribution of width W.

In the uncorrelated limit ($U=0$) this Hamiltonian models the motion of one electron in a disordered lattice. This leads to the problem of Anderson localization,[4] which is now almost understood in the context of a scaling theory.[5] However, the problem of the interplay of disorder and interactions is still a subject of current research where many questions remain unsolved.[5-10] The disordered Hubbard model (also called the Anderson-Hubbard model) has been studied in this context. Kimball[6] gives a qualitative "phase diagram" in the U-W plane, where for large U an insulating phase with a gap in the density of states exists. There is also a gapless phase which is divided in a metallic region (for small W) and a gapless Anderson insulating region. This is confirmed by a real-space renormalization-group calculation of Ma[7] in three dimensions. Shimitzu, Aoki, and Kawimura[8] claim to have developed an improved real-space decimation method, and they calculate the dependence of the gap both with U and W. Also, Allub[9] has performed a thermodynamic study of the model with binary-alloy disorder using a mean-field hopping approximation. The effects of the interactions on the localization properties have also been studied.[10]

Furthermore, it is known that disorder can be an important ingredient in the high-T_c superconductors. There, disorder comes from the oxygen vacancies and the random distribution of holes in the Cu-O planes.[11] Therefore, the study of the Anderson-Hubbard model is also of interest within this context.

In this paper we present results for the Anderson-Hubbard model in the half-filled band case for the paramagnetic phase ($n_\uparrow=n_\downarrow=\frac{1}{2}$). In this case the spectrum for one-particle excitations is symmetric and the Fermi energy lies in the middle of the band ($\mu_F=U/2$). We model the disorder in E_i with a Gaussian distribution of probability

$$P(E_i)=\frac{1}{\sqrt{2\pi}W}e^{-E_i^2/2W^2}\ . \quad (2)$$

We treat the correlations in the alloy-analogy approximation, which is as follows. We think of the propagation of an electron of spin σ as if it were moving in an alloy consisting of two species, in concentrations $n_{\bar{\sigma}}$ and $1-n_{\bar{\sigma}}$, for which the binding energies are E_i+U and E_i, respectively. This analogy would be exact if indeed the $n_{\bar{\sigma}}$ were fixed during the motion of the n_σ. This treatment, for the ordered case, with the coherent-potential approximation (CPA) is equivalent to the "scattering correction" considered by Hubbard [Ref. 1(b)] in the third of a series of papers in this model, and it leads to the exact result in the atomic limit. Recent applications of this alloy-analogy approach in intermediate-valence, heavy-fermion, and high-T_c problems are mentioned in the works of Ref. 12. Note that in the disordered case, we have a problem of a binary alloy superimposed to a continuous distribution of disorder.

Instead of using the CPA, we are going to use a method that we have developed recently,[13] for the calculation of densities of states. This method works in any dimension $d>1$ for hypercubic lattices with diagonal disorder, and it was called the localized-eigenstates approxi-

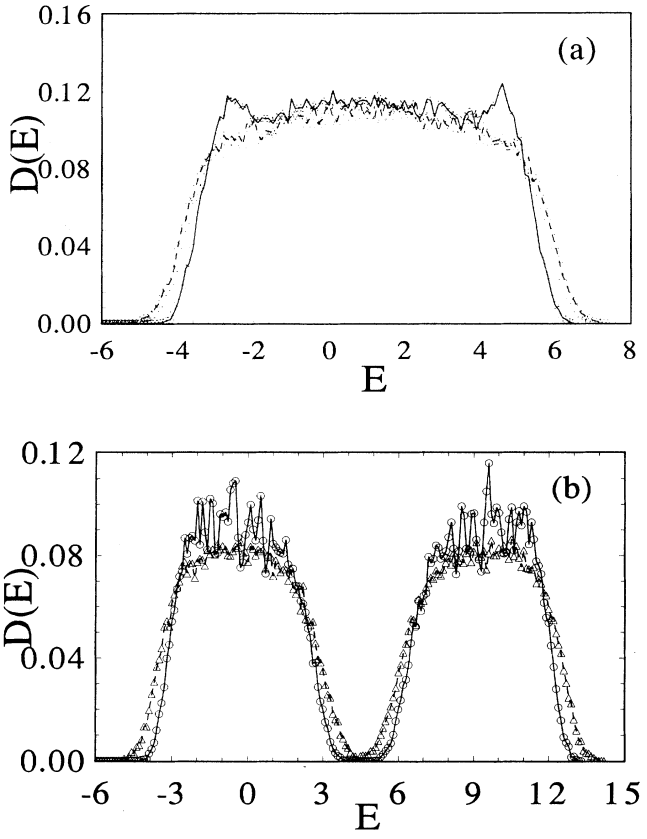

FIG. 1. Densities of states $D(E)$ of the Anderson-Hubbard model in the alloy-analogy approximation, obtained with the LEA. (a) For $U=2$; (b) for $U=9$, a gap opens. ($\circ$, $W=0$; $\triangle$, $W=1$.) The lattice size is $30\times30\times30$. Averages were taken over five disorder configurations.

mation (LEA). It has been compared favorably with exact diagonalization of small three-dimensional (3D) samples of a binary alloy problem.[13] This method is numerically efficient, allowing calculations in large samples. It is also superior to the CPA especially for minority components where the CPA gives very structureless densities of states.

The LEA has been discussed and justified in Ref. 13. It essentially relies on the knowledge (through exact diagonalization) of the eigenvalues in one dimension, and the extension of a dimensional dilution property that is exact in the ordered case. For example, for two dimensions we first diagonalize along chains in, say, the x direction. Then we determine the site of localization with the previous eigenvalues as diagonal energies, and the result comes out as the 2D approximated spectrum.

In Fig. 1 we show the one-particle density of states in the alloy-analogy approximation, calculated with the LEA, both for ordered ($W=0$) and disordered ($W\neq0$) samples of size $30\times30\times30$. (From now on, we give the values of W and U in units of t.) Figure 1(a) shows the case for small U ($U=2$). Clearly, the effect of disorder is to produce a broadening of the band. For a large value of U, a gap opens at the Fermi level, splitting the band in two subbands. An example of this is shown in Fig. 1(b) for $U=9$. In this case, we see that the broadening of the subbands due to the disorder causes a decreasing in the gap width.

To obtain the gap width G as a function of U and W, we use the following procedure. We calculate the distance in energy ΔE between the two eigenvalues closest to the Fermi level $\mu_F=U/2$. Before the opening of a gap ΔE will be of the order of the average separation B/N between energy levels in a finite system, with B the bandwidth and N the size of the system. When ΔE is considerably larger than B/N a gap $G=\Delta E$ will be opened at μ_F. In the inset of Fig. 2(a) we show the behavior of ΔE as a function of U for both 2D and 3D samples. For small U we see that ΔE fluctuates but $\Delta E<B/N$ so there is no gap, and after a certain value of U a gap starts opening. Due to the fluctuations of ΔE in this critical region, it is difficult to define a U_c. We see that for large U the gap increases linearly for both two and three dimensions, and extrapolating this linear behavior to the horizontal axis we can estimate a value of U_c. For two dimensions the U_c for samples of size 30×30, 50×50, and 90×90 is 6.2, 6.0, and 6.0, respectively. In three dimensions samples of size $10\times10\times10$, $20\times20\times20$, and $30\times30\times30$ give $U_c=7.1$, 7.9, and 7.5, respectively. The value of U_c

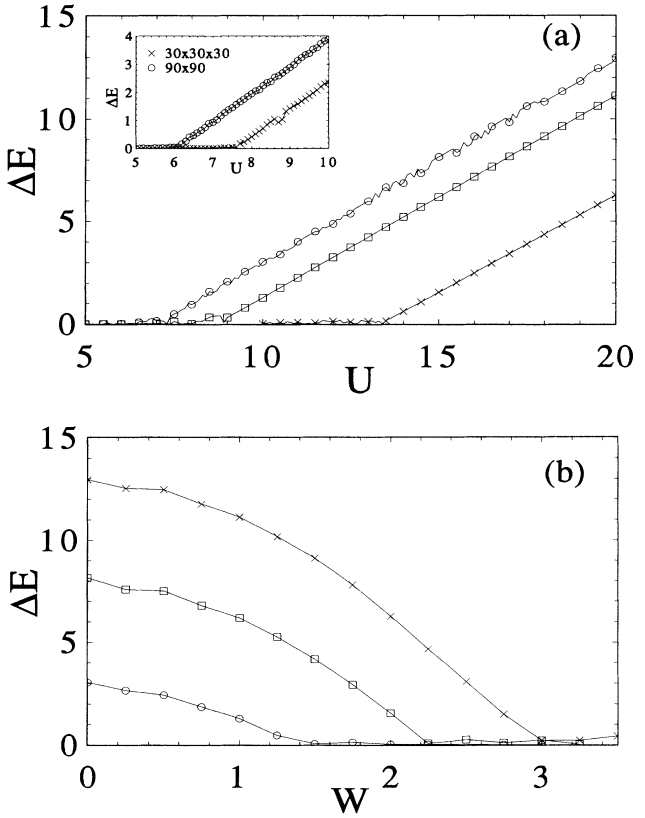

FIG. 2. Behavior of the gap at the Fermi level for lattices of size $10\times10\times10$. (a) As a function of U ($\circ$, $W=0$; $\square$, $W=1$; $\times$, $W=2$). The gap for large 2D (90×90) and 3D ($30\times30\times30$) ordered samples is shown in the inset. (b) Gap as a function of W($\circ$, $U=10$; $\square$, $U=15$; $\times$, $U=20$).

for three dimensions is of the order of the one obtained by Ma[7] and by Shimitzu, Aoki, and Kawimura,[8] although they differ from the value obtained with the Gutzwiller approximation.[14]

The effect of disorder is shown in Fig. 2(a). There we show the gap as a function of U for different values of the disorder. As the disorder reduces the gap, the value of U_c increases with W. Also, it is clear from the plot that the linear growth of the gap with U is independent of the presence of disorder. The behavior of $G \sim (U - U_c)^s$ with $s \approx 1$ in the ordered case ($W = 0$) was also obtained by Ma[7] and by Shimitzu, Aoki, and Kawimura[8] in their real-space renormalization-group calculations. Here we see that this linear relationship also holds in the disordered case.

In Fig. 2(b) we show the behavior of the gap as a function of the disorder W for fixed values of U. The gap decreases due to the broadening of the subbands produced by the disorder, and it tends to disappear at a critical disorder W_c. Also, in this case the gap is $G \sim (W - W_c)^r$ with $r \approx 1$. This linear behavior is in agreement with the results of Shimitzu, Aoki, and Kawimura.[8]

Finally, in Fig. 3 we show the phase diagram of the model in the plane U-W. We have plotted the $U_c(W)$ line obtained by extrapolating the linear behavior of G vs U for different W's. This line separates two phases. For large U there is a phase with a gap at the Fermi level, and therefore it corresponds to a Mott insulator. The other phase below the U_c (W) line is a gapless phase. This phase diagram is similar to the one sketched in the paper by Kimball[6] and to the one calculated by Shimitzu, Aoki, and Kawimura.[8] For low W the U_c line tends to $U_c(0)$ with zero slope. For large W there is an asymptotically linear dependence of $U_c(W)$. It has a slope of $U_c \cong 6.7$ $W (W/t \to \infty)$, which is very close to the fixed point found by Ma[7] for $(t/W, U/W) = (0, 8.3)$. We cannot compare directly with the value of the linear slope obtained by Shimitzu, Aoki, and Kawimura,[8] since in their case they have a uniform probability distribution of disorder instead of a Gaussian disorder, as in our case.

In conclusion, we have found the remarkable fact that the phase diagram obtained with the allow-analogy approximation is very similar to the one obtained with renormalization-group calculations[7,8] for the Anderson-Hubbard model in three dimensions. Also, we have introduced a method for the evaluation of the density of states[13] in the alloy-analogy approach of the Hubbard model, instead of the standard CPA, which is more accurate and gives reasonable results. It remains to separate in the gapless phase the possibility of a metallic behavior or an insulating behavior due to disorder.[6,7] This requires a look at the localization properties of the electronic states at the Fermi level in the gapless phase. There exists the possibility that the eigenstates can be localized in this phase due to the disorder, and hence nonconducting even when the density of states shows no gap. Actually, we expect that this will be the case for W large enough. Therefore, the analysis has to be complemented with a determination of the localization length as a function of the energy. This means to determine the mobility edges in the upper and lower Hubbard bands, obtaining the behavior of a mobility gap as a function of U and W.

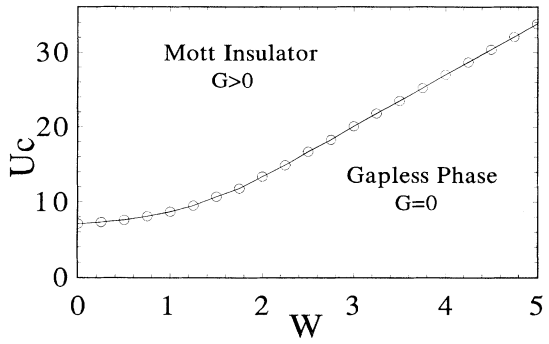

FIG. 3. Phase diagram of the Anderson-Hubbard model. The critical U_c line is plotted as a function of W.

However, this analysis is beyond the LEA method, since this approximation relies on an extension of the localization properties of the eigenstates in one dimension to higher dimensions.[13] Then it cannot give any transition from extended to localized states. We can speculate that in the phase diagram of Fig. 3 the critical line separates between an insulating phase with a gap and an insulating phase with localized states at the Fermi level, at least for $W \gg t$. A metallic phase would also exist below that critical line only for small disorder. Work in this direction, tending to extend the LEA method in order to be able to study localization properties, is in progress.

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